

Superconductivity without Local Inversion Symmetry; Multi-layer Systems

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Abstract.

While multi-layer systems can possess global inversion centers, they can have regions with locally broken inversion symmetry. This can modify the superconducting properties of such a system. Here we analyze two dimensional multi-layer systems yielding spatially modulated antisymmetric spin-orbit coupling (ASOC) and discuss superconductivity with mixed parity order parameters. In particular, the influence of ASOC on the spin susceptibility is investigated at zero temperature. For weak inter-layer coupling we find an enhanced spin susceptibility induced by ASOC, which hints the potential importance of this aspect for superconducting phase in specially structured superlattices.

1. Introduction

The discovery of superconductivity in the non-centrosymmetric heavy Fermion compound CePt₃Si [1, 2] has attracted much attention. Non-centrosymmetry leads to antisymmetric spin-orbit coupling (ASOC) which, for example, gives rise to mixed parity pairing, and the characteristic anisotropy of the spin susceptibility in the superconducting state [3-9].

Recently, artificial superlattices involving the heavy Fermion compound CeIn₃ [10] and CeCoIn₅ [11] have been fabricated, realizing two-dimensional multi-layer structures of heavy electron systems and ordinary metals. A particularly interesting case is the superlattice of CeCoIn₅ and YbCoIn₅ which shows superconductivity, most likely induced by the CeCoIn₅ layers. Motivated by this system we setup a model of a superconductor with similar layered structure, including the fact that such structures show distinctive violation of inversion (reflection) symmetry, while the overall system has inversion centers. Such local non-centrosymmetry is expected to have a pronounced effect on the superconducting phase through local occurrence of ASOC, in particular, for the spin susceptibility.

2. Formulation of model

We introduce here model Hamiltonian for multi-layer systems including ASOC, given by

$$\begin{aligned}
 H = & \sum_{\mathbf{k}, s, m} \varepsilon(\mathbf{k}) c_{\mathbf{k}sm}^\dagger c_{\mathbf{k}sm} + \sum_{\mathbf{k}, s, s', m} \alpha_m \mathbf{g}(\mathbf{k}) \cdot \boldsymbol{\sigma}_{ss'} c_{\mathbf{k}sm}^\dagger c_{\mathbf{k}s'm} \\
 & + \frac{1}{2} \sum_{\mathbf{k}, s, s', m} [\Delta_{ss'm}(\mathbf{k}) c_{\mathbf{k}sm}^\dagger c_{-\mathbf{k}s'm}^\dagger + \text{h.c.}] + \sum_{\mathbf{k}, s, \langle m, m' \rangle} t_\perp c_{\mathbf{k}sm}^\dagger c_{\mathbf{k}sm'}, \quad (1)
 \end{aligned}$$

where $c_{\mathbf{k}sm}$ ($c_{\mathbf{k}sm}^\dagger$) is the annihilation (creation) operator for an electron with spin s on the layer m , and $\sigma_{ss'}$ is the Pauli matrices. The (x, y, z) -axes correspond to the (a, b, c) -axes of the tetragonal crystal.

The first two terms describe the intra-layer dispersion and the ASOC. We consider a square lattice with a tight-binding model, i.e., $\varepsilon(\mathbf{k}) = -2t(\cos k_x + \cos k_y) - \mu$. We choose the unit of energy as $t = 1$ and assume the chemical potential $\mu = -1$. The electron density per site is approximately 0.63. The ASOC term preserves time reversal symmetry through the condition $\mathbf{g}(-\mathbf{k}) = -\mathbf{g}(\mathbf{k})$ and has Rashba structure, which we assume a simple form $\mathbf{g}(\mathbf{k}) = (-\sin k_y, \sin k_x, 0)$. The coupling constants α_m are layer dependent and have opposite sign for layers above and below a center layer. The third term introduces intra-layer Cooper pairing via an off-diagonal mean field. Here $\Delta_{ss'm}(\mathbf{k})$ involves both the spin singlet and triplet components,

$$\Delta_{ss'm}(\mathbf{k}) = \begin{pmatrix} -d_{xm}(\mathbf{k}) + id_{ym}(\mathbf{k}) & \psi_m(\mathbf{k}) + d_{zm}(\mathbf{k}) \\ -\psi_m(\mathbf{k}) + d_{zm}(\mathbf{k}) & d_{xm}(\mathbf{k}) + id_{ym}(\mathbf{k}) \end{pmatrix}, \quad (2)$$

where $\psi_m(\mathbf{k})$ and $\mathbf{d}_m(\mathbf{k})$ are scalar and vector order parameters for the spin-singlet and triplet pairing on layer m , respectively. For simplicity we use an order parameter on phenomenological grounds without resorting to any microscopic model based on a pairing mechanism. To be concrete we use an s-wave order parameter for the singlet and a p-wave order parameter for the triplet pairing, where on symmetry grounds we request $\mathbf{d}_m(\mathbf{k}) \parallel \mathbf{g}(\mathbf{k})$: $\psi_m(\mathbf{k}) = \psi_m$ and $\mathbf{d}_m(\mathbf{k}) = d_m \mathbf{g}(\mathbf{k}) = d_m(-\sin k_y, \sin k_x, 0)$. We choose $|\psi_m|, |d_m| \leq 0.01$, small enough to satisfy the condition $|\Delta_{ss'm}(\mathbf{k})| \ll |\alpha_m| \ll \varepsilon_F$. The dominant order parameter component keeps the same sign over all layers, while the other (subdominant) component adjusts the sign with the ASOC (α_m). The fourth term describes the inter-layer hopping of electrons between nearest-neighbor layers. We assume that the inter-layer hopping t_\perp is smaller than the intra-layer hopping t .

3. Numerical results

We now calculate the spin susceptibility of the multi-layer superconductors with spatially inhomogeneous ASOC, concentrating on the magnetic field direction along the c -axis. The spin susceptibility $\chi = \lim_{H \rightarrow 0} \langle M_s \rangle / H$ is obtained numerically by calculating the magnetization $\langle M_s \rangle$ for a small magnetic field \mathbf{H} . The necessary Zeeman coupling term is given by,

$$H_Z = -\frac{g\mu_B}{2} \sum_{\mathbf{k}, s, s', m} \mathbf{H} \cdot \sigma_{ss'} c_{\mathbf{k}sm}^\dagger c_{\mathbf{k}s'm}, \quad (3)$$

where $g = 2$ and μ_B is the Bohr magneton. First, the Hamiltonian is diagonalized in the presence of a field, introducing the unitary transformation $\hat{C}_{\mathbf{k}}^\dagger = \hat{\Gamma}_{\mathbf{k}}^\dagger \hat{U}^\dagger(\mathbf{k})$ in Nambu-space of M layers, where the quasiparticle operators form a $4M$ -dimensional vector

$$\hat{C}_{\mathbf{k}}^\dagger = (c_{\mathbf{k}\uparrow 1}^\dagger, c_{\mathbf{k}\downarrow 1}^\dagger, c_{-\mathbf{k}\uparrow 1}, c_{-\mathbf{k}\downarrow 1}, \dots, c_{\mathbf{k}\uparrow M}^\dagger, c_{\mathbf{k}\downarrow M}^\dagger, c_{-\mathbf{k}\uparrow M}, c_{-\mathbf{k}\downarrow M}) \quad (4)$$

and analogous for the Bogoliubov quasiparticle operators $\hat{\Gamma}_{\mathbf{k}}^\dagger = (\gamma_{\mathbf{k}1}^\dagger, \gamma_{\mathbf{k}2}^\dagger, \dots, \gamma_{\mathbf{k}4M}^\dagger)$. Thus, the Hamiltonian is

$$H + H_Z = \frac{1}{2} \sum_{\mathbf{k}} \sum_{i=1}^{4M} E_i(\mathbf{k}) \gamma_{\mathbf{k}i}^\dagger \gamma_{\mathbf{k}i}, \quad (5)$$

where $E_i(\mathbf{k})$ are the quasiparticle energies. The magnetization is obtained as,

$$\langle M_s \rangle = \frac{g\mu_B}{2} \sum_{\mathbf{k}} \sum_{i=1}^{4M} [\hat{S}^z(\mathbf{k})]_{ii} f(E_i(\mathbf{k})), \quad (6)$$

where $f(E)$ is the Fermi-Dirac distribution function. The matrix representation of spin operator is defined in the $\hat{\Gamma}_{\mathbf{k}}^\dagger$ basis as

$$\hat{S}^\mu(\mathbf{k}) = \hat{U}^\dagger(\mathbf{k}) \hat{\Sigma}^\mu \hat{U}(\mathbf{k}), \quad (7)$$

with $\hat{\Sigma}^\mu$ the μ -component of the spin operator in the $4M$ -dimensional space.

As concrete examples we discuss the spin susceptibility of bi-layer ($M = 2$) and tri-layer ($M = 3$) systems at $T = 0$. The corresponding coupling constants of ASOC are described as $(\alpha_1, \alpha_2) = (\alpha, -\alpha)$ for bi-layers and $(\alpha_1, \alpha_2, \alpha_3) = (\alpha, 0, -\alpha)$ for tri-layers.

We compare now the two cases: (1) the spin triplet channel is dominant $|d_m| > |\psi_m|$ and (2) the spin singlet channel is dominant $|d_m| < |\psi_m|$. In case (1) the spin susceptibility remains unaffected by the superconducting state, $\chi_s = \chi_n$, because the spin triplet component of the type $\mathbf{d}_m(\mathbf{k}) \propto \mathbf{g}(\mathbf{k}) \perp \hat{z}$ is an equal-spin pairing state with Cooper pair spins along the c -axis. Thus, spin polarization in the superconducting phase is possible without pair breaking. This feature is essentially independent of ASOC and inter-layer hopping as can be seen in Fig.1 for both the bi- and tri-layer systems.

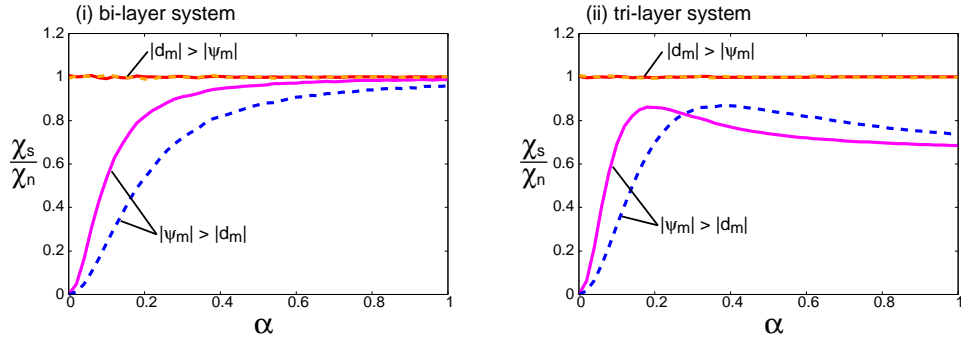


Figure 1. Spin susceptibility along c -axis for bi-layer system (i) and tri-layer system (ii). We assume $t_\perp = 0.1$ (solid line) and $t_\perp = 0.2$ (dashed line).

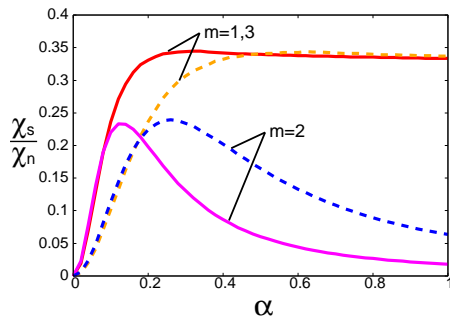


Figure 2. Spin susceptibility along c -axis for tri-layer system. The contribution from each layer is shown. We assume $|\psi_m| > |d_m|$, and $t_\perp = 0.1$ (solid line) and $t_\perp = 0.2$ (dashed line).

More interesting is case (2) as spin singlet pairing leads to complete suppression of the spin susceptibility at $T = 0$ in a conventional superconductor. Indeed for vanishing ASOC ($\alpha = 0$) we find $\chi_s = 0$ irrespective of t_\perp . As soon as ASOC is turned on, however, the spin susceptibility gradually recovers and approaches for large α a constant value: $\chi_s \rightarrow \chi_n$ for the bi-layer and $\chi_s \rightarrow 2\chi_n/3$ for the tri-layer. The mechanism for this behavior lies in the spin-splitting of the electronic spectrum due to the Rashba-type ASOC. The spin polarization involves now an inter-band Van-Vleck-type contribution which is only weakly affected by the opening of quasiparticle

gap in the superconducting phase. Note that this inter-band contribution relies on the ASOC for matrix elements with the Zeeman coupling and is only available for the layers with non-vanishing α . Consequently, in the bi-layer system all layers are involved, giving rise to full recovery of χ_s for large α (analogous to the uniformly non-centrosymmetric superconductor [5]), while in the tri-layer system only two of three layers can contribute yielding a correspondingly reduced limiting value for χ_s . Figure 2 corroborates this picture by considering the contributions of the different layers. Indeed in the large α regime the outer layers $m = 1, 3$ carrying ASOC saturate at $\chi_s \rightarrow \chi_n/3$ while the center layer $m = 2$ completely suppresses. Remarkably at small α ($< t_\perp$), χ_s behaves for all layers in the same way and leads for the center layer to a striking non-monotonic α -dependence.

The numerical data in Fig.1 show that the inter-layer hopping is in competition with ASOC, such that a larger t_\perp yields a higher effective $\alpha_{\text{eff}} \sim t_\perp$ for the crossover from the behavior of conventional superconductor to that of non-centrosymmetric superconductor. This crossover is best evident in the peak of χ_s around $\alpha_{\text{eff}} \sim t_\perp$ for the center layer (Fig.2). Thus, modifying t_\perp , e.g., by uniaxial stress along the c -axis, can influence the magnetic response for c -axis fields in case (2). No such effect is expected for case (1).

Within our model we find that the spin susceptibility along the ab -axis is always the half of the value observed along c -axis, independent of the strength of α and t_\perp and the number of layers. Furthermore, we find that the spin susceptibility for both field directions is affected by the phase difference of order parameter between layers, but independent of the ratio of spin singlet and triplet components. Details will be explained elsewhere.

4. Conclusion

In view of the fact that CeCoIn₅ is known to realize spin singlet superconductivity, we believe that most likely case (2) of our discussion is relevant for the multi-layer systems. Thus, the large observed upper critical fields in the superlattice of CeCoIn₅ [11] would then rely on the presence of the spatially modulated ASOC. Moreover we believe that the variability of the superlattices and also the possibility of local measurements of magnetic properties through NMR would give many intriguing insights into the aspect of ASOC in these artificial systems.

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